Argonne-Northwestern Solar Energy Research (ANSER) Center EFRC Director: Michael R. Wasielewski Lead Institution: Northwestern University

Mission Statement: The mission of the ANSER Center is to revolutionize our understanding of molecules, materials and methods necessary to create dramatically more efficient technologies for solar fuels and electricity production.

The ANSER Center will achieve this vision by understanding and characterizing the basic phenomena of solar energy conversion dynamics, by designing and synthesizing new nanoscale architectures with extraordinary functionality, and by linking basic solar energy conversion phenomena across time and space to create emergent energy conversion systems operating with exceptional performance. At the same time, the ANSER Center seeks to create and mentor a technically excellent workforce capable of solving energy-related problems far into the future. To achieve these goals, ANSER Center objectives are to develop a fundamental understanding of the:

- interaction of light and charge with molecules and materials
- energy levels and electronic structures of molecules and materials
- dynamics of photoinduced charge generation, separation, and transport with unparalleled temporal and spatial resolution
- interfaces at which charge generation, separation, transport, and selective chemical reactions occur
- properties of unique materials, from self-assembling, bio-inspired materials for hydrogen fuel production from water to transparent conductors and nanostructured hard and soft materials for solar electricity generation.

Subtask 1: Bio-inspired molecular materials for solar fuels. Natural photosynthesis is carried out by assemblies of photofunctional chromophores and catalysts within proteins, which provide specifically tailored nano-environments to optimize solar energy conversion. Achieving integrated artificial photosynthetic systems requires hierarchical organization at both molecular and supramolecular levels to capture light energy, separate charge, and transport charge to catalytic sites at which fuel synthesis occurs, e.g., H₂O splitting to generate H₂. We do not yet understand in detail the basic scientific

principles needed to build self-ordering, self-assembling components or the tailored nano-environments necessary to realize efficient, integrated artificial photosynthetic systems. Subtask 1 research targets discovering the fundamental scientific principles necessary to 1) self-assemble biomimetic molecular systems to harvest light and perform photochemical charge separation, 2) couple photogenerated charges to multi-electron, multi-metallic catalysts for H₂O oxidation and

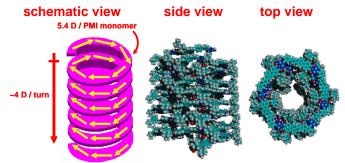


Fig. 1. Self-assembling nano-environment for integrated artificial photosynthesis.

H⁺ reduction to H₂, and 3) develop bio-inspired supramolecular assemblies to produce tailored nanoenvironments necessary for an integrated artificial photosynthetic system (e.g. Fig. 1).

Subtask 2: Interface science of organic photovoltaics. Organic photovoltaics (OPVs) offer the promise of low-cost, readily manufacturable alternatives to traditional inorganic systems for producing solar electricity. Subtask 2 research is directed toward achieving the fundamental understanding required to

achieve power conversion efficiencies as high as 10-15%. Progress requires a highly collaborative group, with experts in transparent conducting oxides (TCOs), in tailoring their interfaces with soft matter, in supramolecular assembly of charge-transporting arrays, and in applying an arsenal of state-of-the-art physical characterization and theoretical techniques. Subtask 2 combines unique, complementary expertise and resources, attacking key problems in OPV interface science in a comprehensive, integrated fashion, to achieve prototype cells which test enabling new concepts (e.g. Fig. 2). The resulting knowledge, materials, and techniques are also exploited in the other types of interfaces necessary to implement the photodriven catalysts and solar cells in Subtasks 1 and 3, respectively.

Subtask 3: Nanostructured architectures for photovoltaic and photochemical energy conversion. This subtask defines, develops, models, and tests robust new nanostructured architectures, and associated new synthetic methodologies, that promise to advance substantially the science and technology of photovoltaic and photochemical solar energy conversion. Specifically, Subtask 3 focuses on high surface area inorganic architectures capable of addressing key challenges in the design of exceptionally efficient Dye Sensitized Solar Cells (DSSCs) and highly functional fuel-producing solar cells (Subtask 1). This work builds on many of the activities in Subtasks 1 and 2 and synergistically provides information back to these subtasks. DSSCs represent one of the most promising alternatives to expensive silicon technology for conversion of solar radiation to electricity (Fig. 3a). Specifically, we are using new materials synthesis techniques to create conducting, semiconducting, and insulating

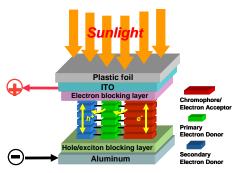


Fig. 2. A multilayer organic solar cell.

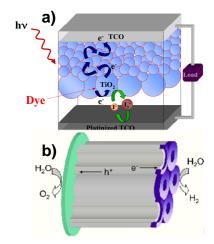


Fig. 3. a) DSSC based on electron injection into a wide bandgap, nanocrystalline, n-type semiconductor. **b)** *Compartmentalized* lightharvesting, catalytic oxidation, and catalytic reduction components function on a higharea, high-porosity, electrically conductive platform.

oxide and metal nanostructures that can be used to systematically control key electronic, catalytic, and optical phenomena, and to favorably manipulate device dynamics and energetics. These structures enable the plasmonic amplification of light harvesting ability, the use of energetically optimized redox shuttles that do not work in conventional architectures, and the coupling of photoelectrodes to fuelforming catalysts (Fig. 3b).

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